

ADVANCED SIMULATIONS OF BIOMATERIALS: FROM ATOMISTIC TO MESOSCALE SIMULATIONS

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ABSTRACT

The main focus of this invited session is on elucidating the biomechanical behavior of tissues, cells, and biomolecules through the use of novel computational techniques. The significance of cells and tissues as the main building blocks of human body from one side and the role of biomechanical reactions such as cell growth, proliferation, differentiation, motility, and apoptosis on the fate of cells from the other side, makes the study of their biomechanical behavior prominent. However, the traditional tools such as finite element methods usually fail at this length space. Thus, this invited session aims to discuss the recent advances in the use of various computational tools from atomistic to mesoscale simulations in this realm. Specially interesting would be the use of models that investigate the interface between various biological entities. The involved interfaces usually include the interaction of soft materials with hard materials which are challenging to model since the methods deployed in modeling these two categories are not compatible. Another area of interest would be the discovery of the interface structure since there are limited information in this regard despite their significant influence on the predictions done by the simulations.

Topics of interest for this invited session are:

- The use of novel computational techniques in the studying the molecules, cells and tissues properties.
- Multi-scale simulations of biomaterials.
- Novel techniques in unraveling the interfaces in the biological entities.